

Modified atomic orbital calculations for $(1s, nl)^3L^\pi$ and ${}_2(1,0)_n^{\pm 1,3}S^e$ excited states of He isoelectronic sequence

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Abstract. The singly $(1s, ns)^3S^e$, $(1s, np)^3P^o$, $(1s, nd)^3D^e$ excited states and the doubly ${}_2(1,0)_n^+S^e$ and ${}_2(1,0)_n^-S^e$ ($n \leq 10$) autoionizing states of the helium isoelectronic sequence are investigated using Modified Atomic Orbital Theory (MAOT). Total energies up to $Z = 10$ and excitation energies with $Z = 2 \sim 5$ are presented and comparison with experimental and theoretical available results indicates a good agreement. In addition, the method is applied in the calculation of accurate results in very high Z - He isoelectronic sequence with $11 \leq Z \leq 58$ and with $Z = 60, 70, 80, 90, 91$ and 92 for the $(1s, ns)^1,3S^e$, $(1s, np)^1,3P^o$, $(1s, nd)^1,3D^e$, ${}_2(1,0)_n^+S^e$ and ${}_2(1,0)_n^-S^e$ ($n \leq 7$) excited states. The results obtained for these high Z - He isoelectronic sequence are in good agreement with double sums over the complete hydrogen spectrum calculations of Ivanov and Safronova.

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Key words: atomic orbital theory, screening constant, semi-empirical calculations, autoionizing, excited states, helium isoelectronic sequence

1 Introduction

Studies of excited states in two electron systems remain an active field of research both experimentally and theoretically since the earlier synchrotron radiation source experiment of Madden and Codling on He [1]. At present moment, the description of the properties of the excited states in the helium isoelectronic series is done in the framework of the new classification scheme with the label ${}_n(K, T)_N^A 2S^{+1}L^\pi$. In this notation, N and n denote respectively the principal quantum numbers of the inner and of the outer electron, S the total spin, L the total angular momentum, π the parity of the system, K and T are angular correlation quantum numbers and A represents the radial correlation quantum

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number of the two electrons. Besides, this designation incorporates singly excited states and both intrashell and intershell excited states in the helium-like ions. A given channel μ is labelled by: $\mu = (K, T)_N^A 2^{S+1} L^\pi$, as originally used by Herrick and Sinanoglu [2, 3] with the following assignment of K and T for a given N , L and π

$$T = 0, 1, 2, \dots, \min(L, N-1),$$

$$K = N-1-T, N-3-T, \dots, -(N-1-T).$$

These assigned values of K and T depend not on the total angular spin S . Besides, T is roughly speaking the projection of L onto the interelectronic axis and describes then the orientations between the orbitals of the two electrons and K is related to the cosinus of the interelectronic angle as: $K \approx -\langle r_{<} \cos \theta_{12} \rangle$, where $r_{<}$ denotes the radius of the inner electron. Physically, the larger the positive value of K , the value of $-\langle \cos \theta_{12} \rangle$ is closer to unity. In addition, A can take the values $+1$ or -1 and 0 only [4]. For the $A=+1$ states, the two electrons tend to approach or to move away from the nucleus in phase and for $A=-1$ states, the two electrons have out- of-phase such that, when one electron approaches the nucleus, the other tends to move away from it [5]. For $A=0$ states, they are little radial correlation between the two electrons and they are similar to singly excited states [4].

For the lowest-energy envelope ($N=1$) containing the $(1s, nl)^{2S+1} L^\pi$ singly-excited states and for the ${}_2(1,0)_n^{+1} S^e$ and ${}_2(1,0)_n^{-3} S^e$ doubly excited states, various methods of calculation are used, such as the hyperspherical close-coupling method [6], the double sums over the total hydrogen spectrum of product of radials integrals technique [7], the analytical method [8], the spin-dependent localized Hartree-Fock density-functional theory [9], the truncated diagonalization technique [10], the saddle-point complex-rotation method [11], the close-coupling method [12], the discretization technique [13], the complex-coordinate rotation [14–16], the density functional theory [17], and so on.

Recently, we have presented a modification of the atomic orbital theory of Slater (MAOT) and applied it successfully to the calculation of energies for $(1sns)^1 S^e$, $(1snp)^1 P^o$, $(1snd)^1 D^e$ and $(ns^2)^1 S^e$, $(np^2)^1 D^e$, $(nf^2)^1 I^e$, $(nh^2)^1 K^e$ excited states of He-like ions up to $Z=12$ [18]. In the present paper, we extend these calculations in the case of the singly $(1s, ns)^3 S^e$, $(1s, np)^3 P^o$, $(1s, nd)^3 D^e$ and of the doubly ${}_2(1,0)_n^{+1} S^e$ and ${}_2(1,0)_n^{-3} S^e$ ($n \leq 10$) excited states of the helium isoelectronic sequence. Calculations are performed for total energies up to $Z=10$ and excitation energies with $Z=2 \sim 5$ and compared to experimental and theoretical available results. In addition, the method referred as MAOT is applied in the calculation of accurate results in very high Z - He isoelectronic sequence with $11 \leq Z \leq 58$ and with $Z=60, 70, 80, 90$ and 92 for the $(1s, ns)^{1,3} S^e$, $(1s, np)^{1,3} P^o$, $(1s, nd)^{1,3} D^e$, ${}_2(1,0)_n^{+1} S^e$ ($n \leq 7$) excited states. For these high Z - He -like ions, only the theoretical results from double sums over the complete hydrogen spectrum method of Ivanov and Safronova [7] with $n \leq 4$ are available. Comparison with respect to the forecast of these authors is then made.